

"Linked cluster expansion" for Ω

(1)

$$\hat{H} = \hat{H}_0 + \underbrace{\hat{H}'}_{\text{interactions}}$$

TD potential

$$\Omega = -T \text{Tr} \langle e^{-\beta \hat{H}} \rangle$$

Interaction representation

$$\Omega - \Omega_0 = -T \log \langle U(\tau) \rangle$$

where $U(\tau) = \underbrace{\hat{T}_\tau}_{\tau\text{-ordering}} \exp \left(- \int_0^\beta \hat{H}'(\tau) d\tau \right)$ - evolution operator

Consider at first $\langle U(\tau) \rangle$, Taylor expansion reads

$$\langle U(\tau) \rangle = \sum_n \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \dots d\tau_n \langle \hat{T}_\tau [\hat{H}'(\tau_1) \dots \hat{H}'(\tau_n)] \rangle$$

Example: e-ph interactions

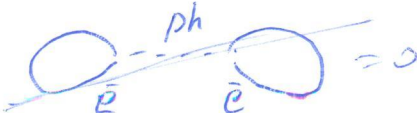
$$\hat{H}' = \sum_{p,q} \frac{M_q}{\sqrt{V}} \hat{A}_q \hat{C}_{p+q}^\dagger \hat{C}_p$$

$\hat{C}^\dagger, \hat{C}$ - fermionic

$\hat{A}_q$ - bosonic

M_q - interaction matrix element

Note: $\langle \hat{A}_q^{2n+1} \rangle = 0$. Apply the Wick theorem

$\hat{A}^2$  = 0 $\bar{e}$  $\bar{e}$ - closed loop

$\hat{A}^4$ 1)  2)  3)  4) 

2-4 - connected diagram (none of $\hat{H}'(\tau_i)$ is missed during successive pairing of operators) 2

1) - disconnected diagrams

Let's find combinatorial factors

Consider given n

$$\frac{(-1)^n}{n!} \int_0^{\beta} d\tau \{\epsilon\} \langle \hat{T}_\tau [\underbrace{\hat{H}' \dots \hat{H}'}_{\tau_1 \rightarrow \tau_n - \text{labeled times}}] \rangle$$

1) Select a diagram with given number of loops k and given structure of all loops

$$\frac{(-1)^n}{n!} \int d\tau \{\epsilon\} \langle \hat{T}_\tau [\underbrace{\hat{H}' \dots \hat{H}'}_{\tau_1^{(1)} \rightarrow \tau_{m_1}^{(1)}}] \rangle_c \int d\tau_2 \{\epsilon\} \langle \hat{T}_\tau [\underbrace{\hat{H}' \dots \hat{H}'}_{\tau_1^{(2)} \rightarrow \tau_{m_2}^{(2)}}] \rangle_c \dots \int d\tau_k \{\epsilon\} \langle \hat{T}_\tau [\underbrace{\hat{H}' \dots \hat{H}'}_{\tau_1^{(k)} \rightarrow \tau_{m_k}^{(k)}}] \rangle_c \quad (1)$$

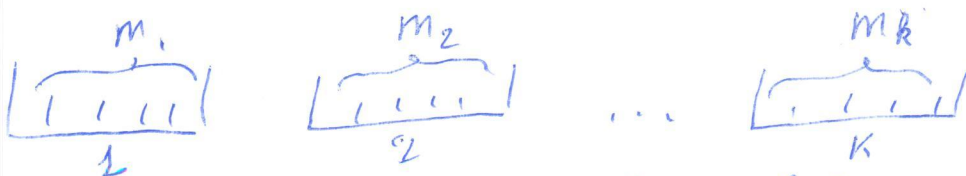
(c) - Connected

where $\{m_j\}$ - number in interaction vertices

Start with the case of different $m_1 \neq m_2 \neq \dots m_k$

Note $\sum m_j = k$

Combinatorics ① ② ... ① - labeled balls



How many ways to distribute balls over boxes?

Answer $F_k = \frac{n!}{m_1! m_2! \dots m_k!}$ - polynom. / coefficient

rewrite Eq(1) as follows

3

$$\frac{n!}{n!} \prod_{i=1}^k \left[\frac{(-1)^{m_i}}{m_i!} \int d^{m_i} \{ \tau \} \langle \hat{T}_\tau [\hat{H}'_{\tau_1^{(1)} \rightarrow \tau_{m_1}^{(1)}} \dots \hat{H}'_{\tau_i^{(i)} \rightarrow \tau_{m_i}^{(i)}}] \rangle_c \right] \quad (2)$$

2) Generalize (2)

let $\langle \dots \rangle_{c-all}$ denote a sum of all connected diagrams with given number of vertices (m_i are still different)

Introduce

$$\Xi_m = \frac{(-1)^m}{m!} \int d^m \{ \tau \} \langle \hat{T}_\tau [\hat{H}'_{\tau_1^{(1)} \rightarrow \tau_m^{(1)}} \dots \hat{H}'_{\tau_m^{(m)} \rightarrow \tau_m^{(m)}}] \rangle_{c-all}$$

("c-all" will be omitted below)

Summing all different loops (i.e., $\langle \dots \rangle_c \rightarrow \langle \dots \rangle_{c-all}$) we obtain

$$\prod_{j=1}^k \Xi_{m_j} \quad (3)$$

Note important property

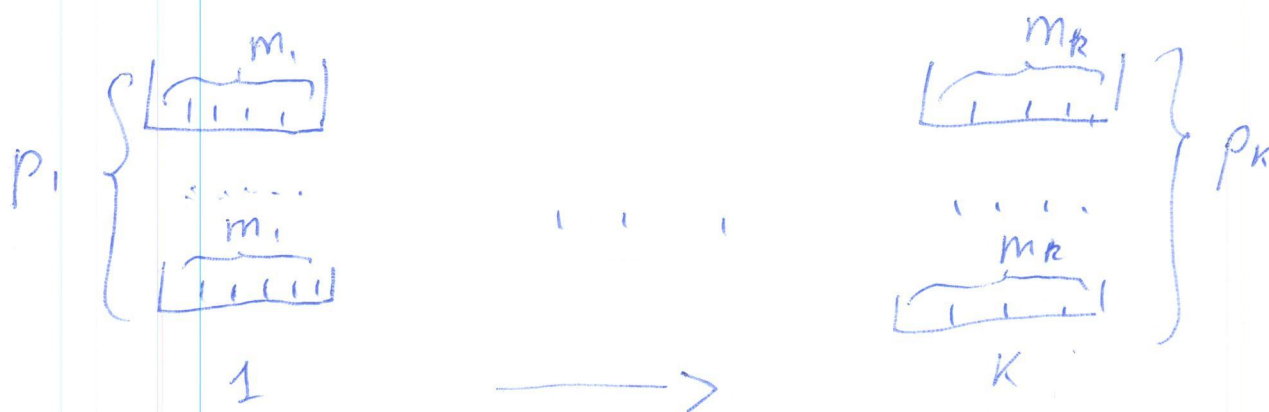
$$\sum_{m=0}^{\infty} \Xi_m \equiv \langle U(\beta) \rangle_c$$

$$(\Xi_0 \equiv 1)$$

3) Generalize (3) for the case, where some m_i are equal to each other: introduce "degeneracy factors" p_i , so that the Wick theorem each time yields $\sum_{j=1}^k p_j$ loops.

Note that generically $n = \sum_i m_i p_i$

Combinatorics ① ② ... ④ - labelled balls



How many ways to distribute?

Answer $\bar{F}_R = \frac{n!}{p_1! (m_1!)^{p_1} p_2! (m_2!)^{p_2} \dots p_k! (m_k!)^{p_k}}$

$\Rightarrow$ (3) can be generalized as follows

$$\mathcal{Z}(\{p_i\}) = \prod_{j=1}^k \left[\frac{1}{p_j!} \left(\sum_{m_j} \right)^{p_j} \right] \quad \text{or}$$

$$\frac{1}{p_1!} \left(\sum_1 \right)^{p_1} \frac{1}{p_2!} \left(\sum_2 \right)^{p_2} \dots \frac{1}{p_\ell!} \left(\sum_\ell \right)^{p_\ell}$$

factors for loops of order ℓ in the whole diagram

Regrouping the series

$$\begin{aligned}
 \langle U(\beta) \rangle &= \sum_{\{p_i\}} \frac{1}{p_1!} (\Xi_1)^{p_1} \frac{1}{p_2!} (\Xi_2)^{p_2} \dots = \\
 &= \sum_{p_1} \frac{1}{p_1!} (\Xi_1)^{p_1} \sum_{p_2} \frac{1}{p_2!} (\Xi_2)^{p_2} \dots = \\
 &= \text{|| recall property of } \Xi_m \text{ || } e^{\Xi_1} e^{\Xi_2} \dots = \\
 &= e^{\Xi_1 + \Xi_2 + \dots} = e^{\langle U(\beta) \rangle_c - 1}
 \end{aligned}$$

Thus $\Omega - \Omega_c = -T \log \langle U(\beta) \rangle = -T (\langle U(\beta) \rangle_c - 1)$